



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 99104

TO: Robert Mondesi
Location: CM1/5D16&9B01
Art Unit: 1653
July 29, 2003

Case Serial Number: 09/825399

From: P. Sheppard
Location: CM1-1E03
Phone: (703) 308-4499

sheppard@uspto.gov

Search Notes

99104

Access DB# _____

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Robert Mondesi Examiner #: 79912 Date: _____
Art Unit: 1653 Phone Number 305-4445 Serial Number: 09825399
Mail Box and Bldg/Room Location: _____ Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

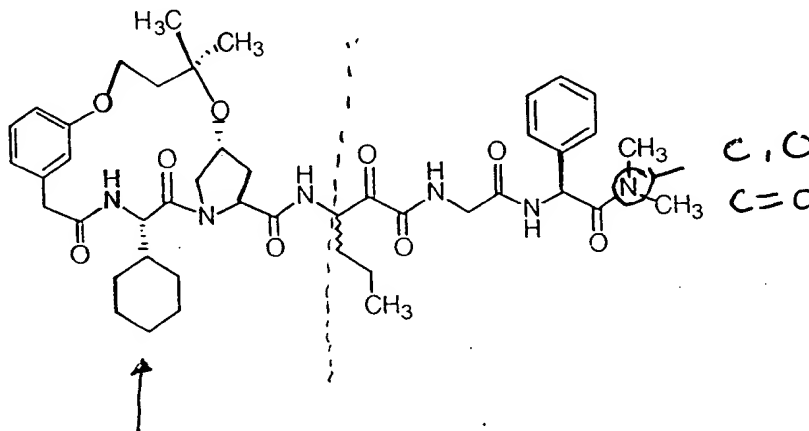
Title of Invention: Macrocyclic NS3-serine protease inhibitors of hepatitis C

Inventors (please provide full names):

Chen, Kevin X; Araseppan, Ashok; Venkatraman, Srikant

Earliest Priority Filing Date: 4-20-2001

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



Core structure
must remain
constant.

Search for
variables.

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 18:56:50 ON 29 JUL 2003

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FILE COVERS 1907 - 29 Jul 2003 VOL 139 ISS 5

FILE LAST UPDATED: 28 Jul 2003 (20030728/ED)

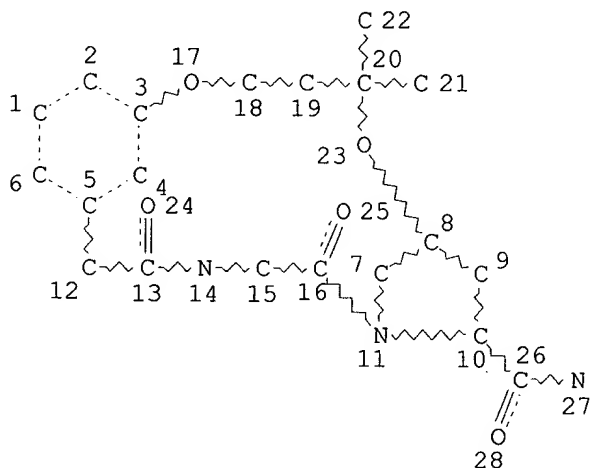
This file contains CAS Registry Numbers for easy and accurate substance identification.

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L1 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

L3 33 SEA FILE=REGISTRY SSS FUL L1

L4 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

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=>

=> d ibib abs hitrn 14 1

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2001:763001 HCAPLUS
 DOCUMENT NUMBER: 135:318715
 TITLE: Preparation of macrocyclic NS3-serine protease inhibitors of hepatitis C virus comprising n-cyclic p2 moieties
 INVENTOR(S): Chen, Kevin X.; Arasappan, Ashok; Venkatraman, Srikanth; Parekh, Tejal N.; Gu, Haining; Njoroge, F. George; Girijavallabhan, Viyyoor M.; Ganguly, Ashit; Saksena, Anil; Jao, Edwin; Yao, Nanhua H.; Prongay, Andrew J.; Madison, Vincent S.; Vibulbhan, Banacha
 PATENT ASSIGNEE(S): Schering Corporation, USA
 SOURCE: PCT Int. Appl., 402 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077113	A2	20011018	WO 2001-US10869	20010403
WO 2001077113	A3	20020620		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002107181	A1	20020808	US 2001-825399	20010403
EP 1268525	A2	20030102	EP 2001-926601	20010403
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001009861	A	20030610	BR 2001-9861	20010403
NO 2002004797	A	20021204	NO 2002-4797	20021004
PRIORITY APPLN. INFO.: US 2000-194607P P 20000405				
WO 2001-US10869 W 20010403				
OTHER SOURCE(S): MARPAT 135:318715				
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [wherein X and Y = independently (cyclo)alkyl, heteroalkyl, (aryl)heteroaryl, alkyl(hetero)aryl, substituted ether, sulfide, sulfone, amide, sulfonamide, urea, carbamate, hydrazide, carbonyl, etc.; R1 = CHO, acyl, or (un)substituted carboxy, carbamoyl, boryl, etc.; Z = O, N, or CH, W = null or CO, CS, or SO2; Q = null or CH, N, P, (CH2)p, (CHR)p, (CRR')p, O, NR, S, or SO2; A = O, CH2, (CHR)p, (CHRCHR')p, (CRR')p, NR, S, SO2, or a bond; E = CH, N, CR, or a double bond toward A, L, or G; G = null or (CH2)p, (CHR)p, or (CRR')p; J = null or CH, CR, O, S, or NR; M = null or O, NR, S, SO2, "(CH2)p, (CHR)p, (CHRCHR')p, or (CRR')p; p = 0-6; R, R', R2, R3, and R4 = independently H, (cyclo)alkyl, alkenyl, heterocycloalkyl, alkoxy, aryloxy, alkylthio, arylthio, amino, amido, ester, carboxylic acid, carbamate, urea, ketone,

CHO, CN, NO₂, O, N, S, P, etc.] were prepd. as hepatitis C virus (HCV) protease inhibitors. For example, II (multi-step prepn. given) was cyclized, deesterified, and coupled with III.bul.HCl (prepn. given) to give the macrocyclic hydroxyamide intermediate. Oxidn. using Des-Martin reagent followed by flash chromatog. afforded two diastereomers IV in 82% combined yield. The (S)-isomer inhibited NS3-serine protease HeLa/Huh7 co-transfected cells with a K_i of 2 .mu.M. The invention also discloses pharmaceutical compns. comprising I as well as methods of using them to treat disorders assocd. with the HCV protease.

IT 367257-61-2P 367257-62-3P 367257-96-3P
 367258-03-5P 367258-08-0P 367258-09-1P
 367258-10-4P 367258-11-5P 367258-12-6P
 367258-13-7P 367258-14-8P 367258-15-9P
 367258-16-0P 367258-17-1P 367258-18-2P
 367258-19-3P 367258-20-6P 367258-21-7P
 367258-22-8P 367258-23-9P 367258-24-0P
 367258-25-1P 367258-26-2P 367258-27-3P
 367258-28-4P 367258-29-5P 367258-30-8P
 367258-31-9P 367258-32-0P 367258-33-1P
 367258-34-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of macrocyclic NS3-serine protease inhibitors of hepatitis C virus comprising cyclic p2 moieties)

IT 368871-35-6P 368871-36-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of macrocyclic NS3-serine protease inhibitors of hepatitis C virus comprising cyclic p2 moieties)

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=> fil reg

FILE 'REGISTRY' ENTERED AT 18:57:06 ON 29 JUL 2003

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 JUL 2003 HIGHEST RN 556740-18-2

DICTIONARY FILE UPDATES: 28 JUL 2003 HIGHEST RN 556740-18-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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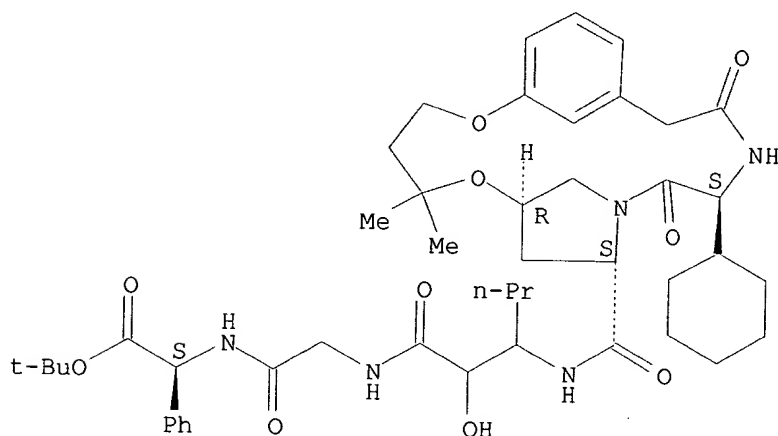
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=> d ide can 13 1-33

L3 ANSWER 1 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 368871-36-7 REGISTRY
 CN Glycine, (2S)-2-cyclohexyl-N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]glycyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-hydroxyhexanoylglycyl-2-phenyl-, 1,1-dimethylethyl ester, cyclic (1.fwdarw.2)-ether, (2S)- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C46 H65 N5 O10
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

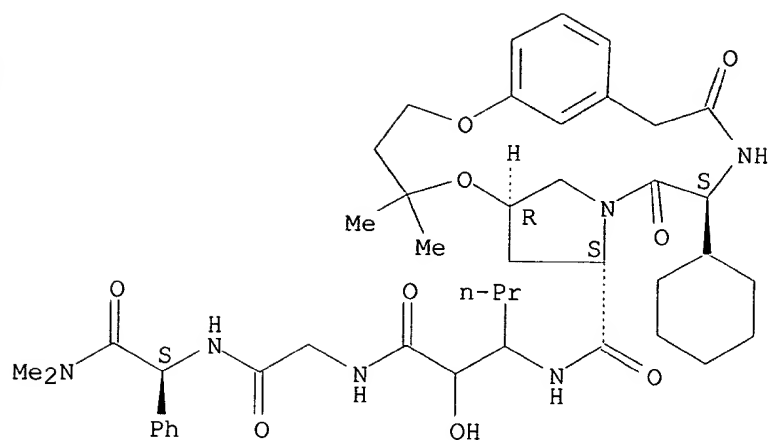
1 REFERENCES IN FILE CA (1947 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 2 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 368871-35-6 REGISTRY
 CN Glycinamide, (2S)-2-cyclohexyl-N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]glycyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-hydroxyhexanoylglycyl-N,N-dimethyl-2-phenyl-, cyclic (1.fwdarw.2)-ether, (2S)- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C44 H62 N6 O9
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



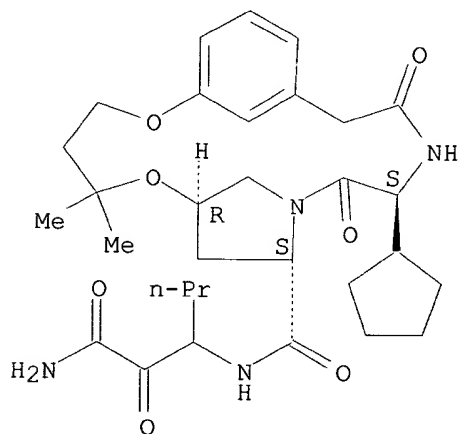
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1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 3 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-34-2 REGISTRY
CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, N-[1-(aminooxoacetyl)butyl]-12-cyclopentyl-5,5-dimethyl-11,14-dioxo-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H44 N4 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



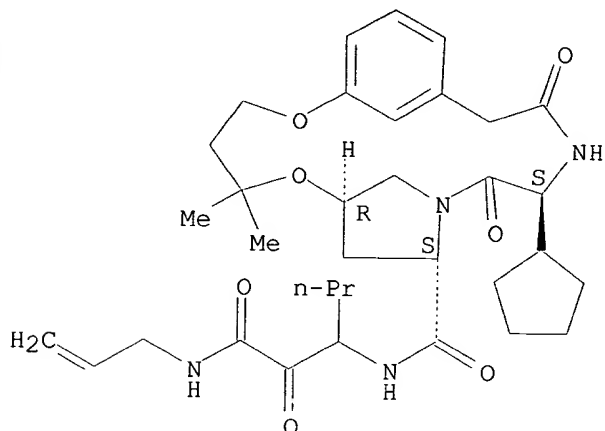
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1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 4 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367258-33-1 REGISTRY
 CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, 12-cyclopentyl-5,5-dimethyl-11,14-dioxo-N-[1-[oxo(2-propenylamino)acetyl]butyl]-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C34 H48 N4 O7
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



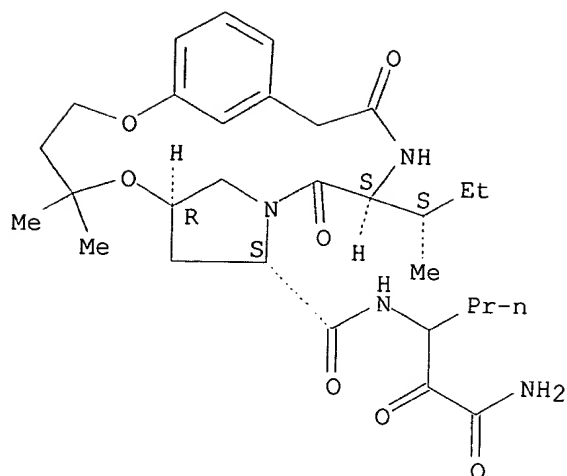
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1 REFERENCES IN FILE CA (1947 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 5 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367258-32-0 REGISTRY
 CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, N-[1-(aminooxoacetyl)butyl]-5,5-dimethyl-12-[(1S)-1-methylpropyl]-11,14-dioxo-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C30 H44 N4 O7
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



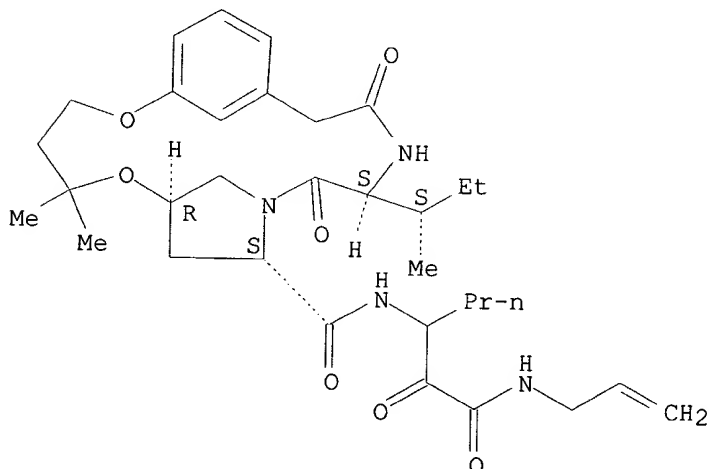
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1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 6 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-31-9 REGISTRY
CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, 5,5-dimethyl-12-[(1S)-1-methylpropyl]-11,14-dioxo-N-[1-[oxo(2-propenylamino)acetyl]butyl]-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H48 N4 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

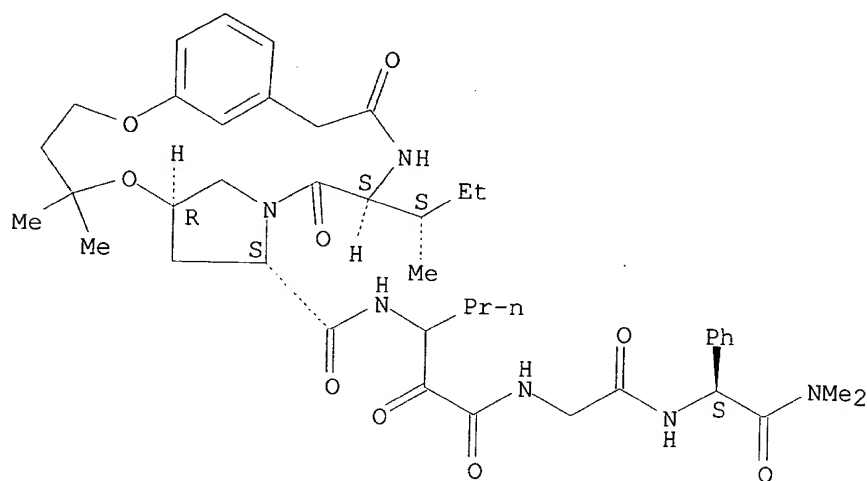
1 REFERENCES IN FILE CA (1947 TO DATE)

1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 7 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367258-30-8 REGISTRY
 CN Glycinamide, N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]-L-isoleucyl-
 (4R)-4-hydroxy-L-prolyl-3-amino-2-oxohexanoylglycyl-N,N-dimethyl-2-phenyl-
 , cyclic (1.fwdarw.2)-ether, (2S)- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C42 H58 N6 O9
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



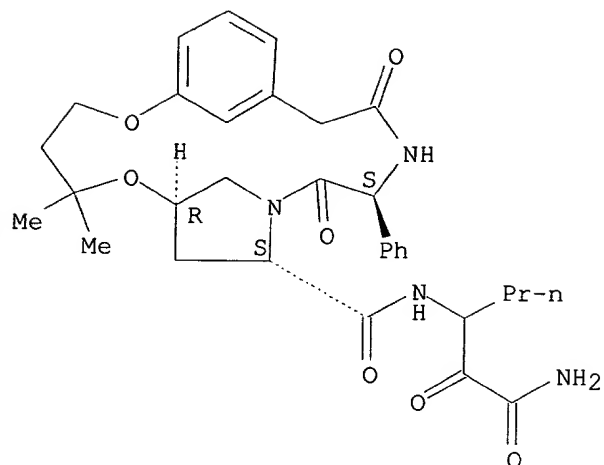
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1 REFERENCES IN FILE CA (1947 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 8 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367258-29-5 REGISTRY
 CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-
 carboxamide, N-[1-(aminooxoacetyl)butyl]-5,5-dimethyl-11,14-dioxo-12-
 phenyl-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C32 H40 N4 O7
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



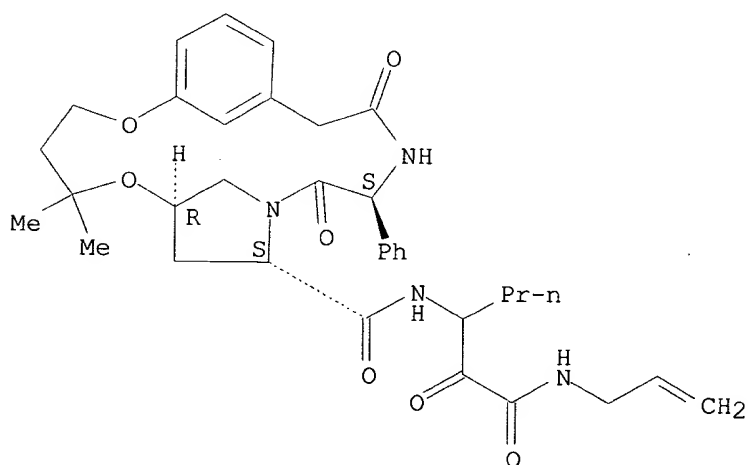
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1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 9 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-28-4 REGISTRY
CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, 5,5-dimethyl-11,14-dioxo-N-[1-[oxo(2-propenylamino)acetyl]butyl]-12-phenyl-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C35 H44 N4 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



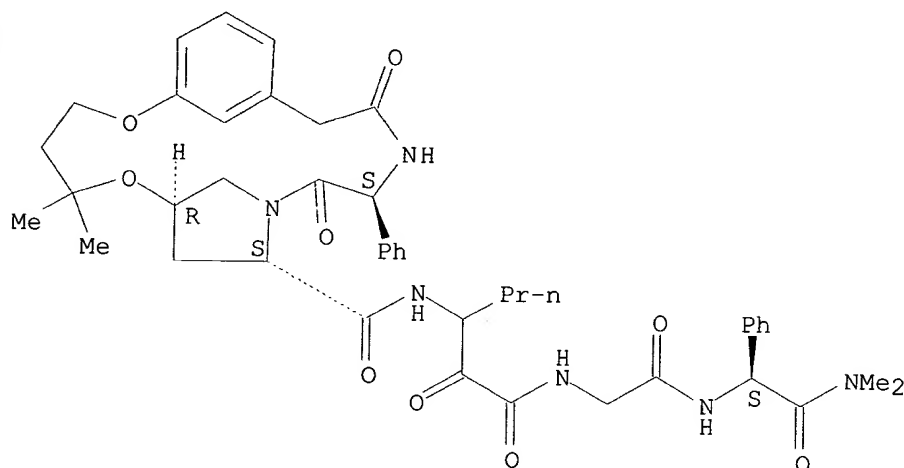
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1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 10 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-27-3 REGISTRY
CN Glycinamide, (2S)-N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]-2-phenylglycyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-oxohexanoylglycyl-N,N-dimethyl-2-phenyl-, cyclic (1.fwdarw.2)-ether, (2S)- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C44 H54 N6 O9
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



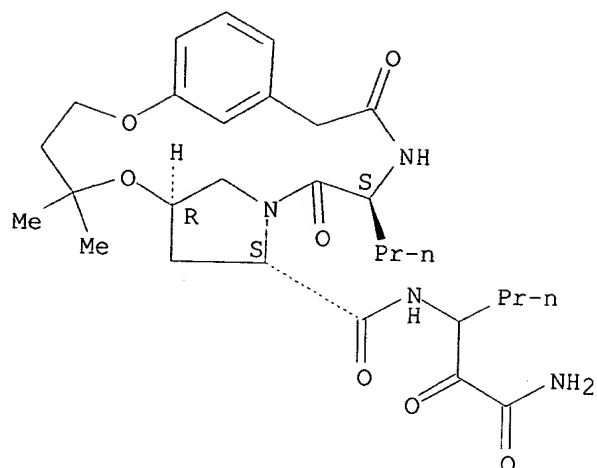
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1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 11 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-26-2 REGISTRY
CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, N-[1-(aminooxoacetyl)butyl]-5,5-dimethyl-11,14-dioxo-12-propyl-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H42 N4 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



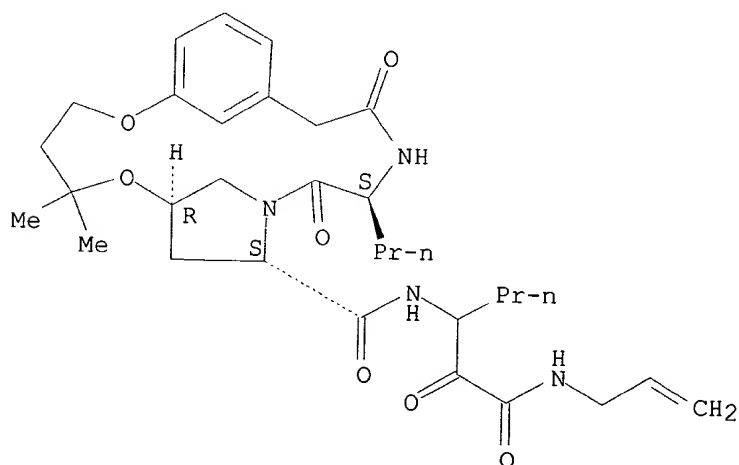
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1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 12 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-25-1 REGISTRY
CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, 5,5-dimethyl-11,14-dioxo-N-[1-[oxo(2-propenylamino)acetyl]butyl]-12-propyl-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H46 N4 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



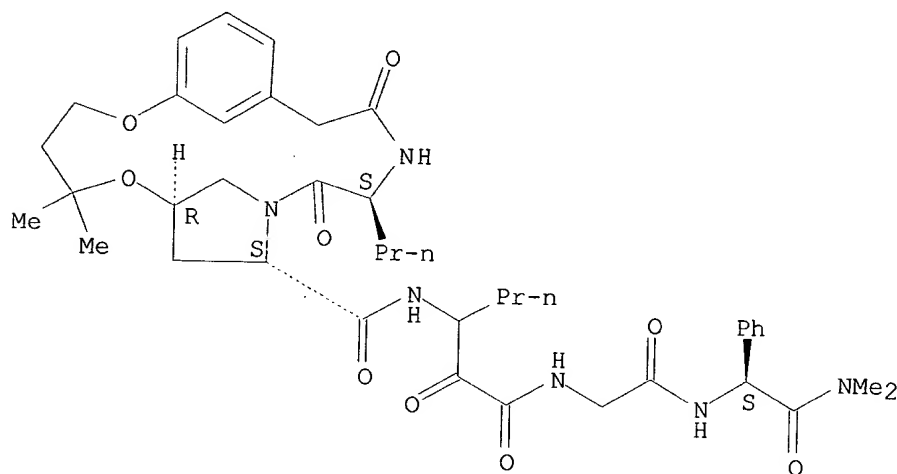
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1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 13 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-24-0 REGISTRY
CN Glycinamide, N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]-L-norvalyl-
(4R)-4-hydroxy-L-prolyl-3-amino-2-oxohexanoylglycyl-N,N-dimethyl-2-phenyl-
, cyclic (1.fwdarw.2)-ether, (2S)- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
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SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



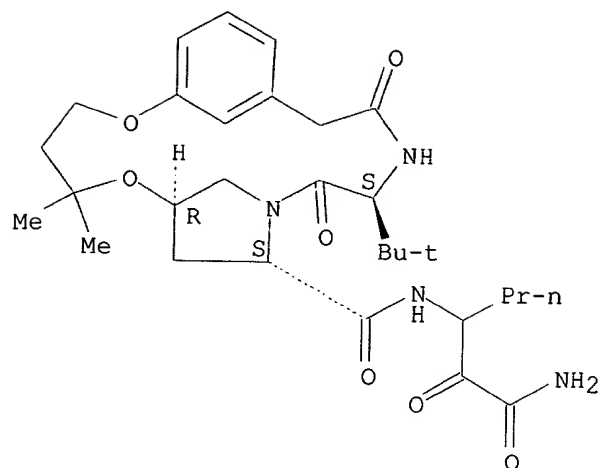
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REFERENCE 1: 135:318715

L3 ANSWER 14 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-23-9 REGISTRY
CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-
carboxamide, N-[1-(aminooxoacetyl)butyl]-12-(1,1-dimethylethyl)-5,5-
dimethyl-11,14-dioxo-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
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LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



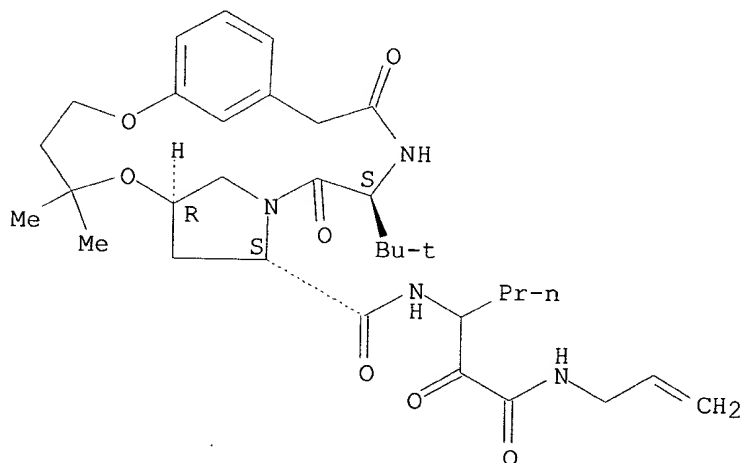
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1 REFERENCES IN FILE CA (1947 TO DATE)
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REFERENCE 1: 135:318715

L3 ANSWER 15 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-22-8 REGISTRY
CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, 12-(1,1-dimethylethyl)-5,5-dimethyl-11,14-dioxo-N-[1-[oxo(2-propenylamino)acetyl]butyl]-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H48 N4 O7
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LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)

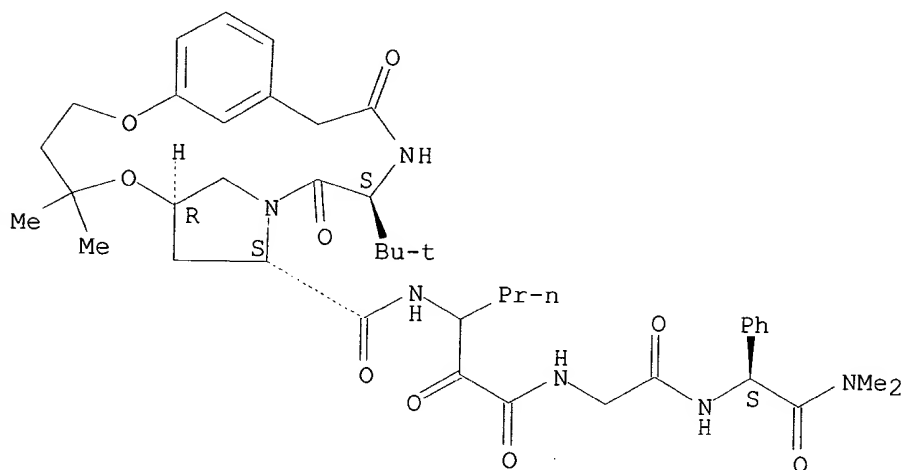
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 16 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
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 CN Glycinamide, N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]-3-methyl-L-valyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-oxohexanoylglycyl-N,N-dimethyl-2-phenyl-, cyclic (1.fwdarw.2)-ether, (2S)- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C42 H58 N6 O9
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



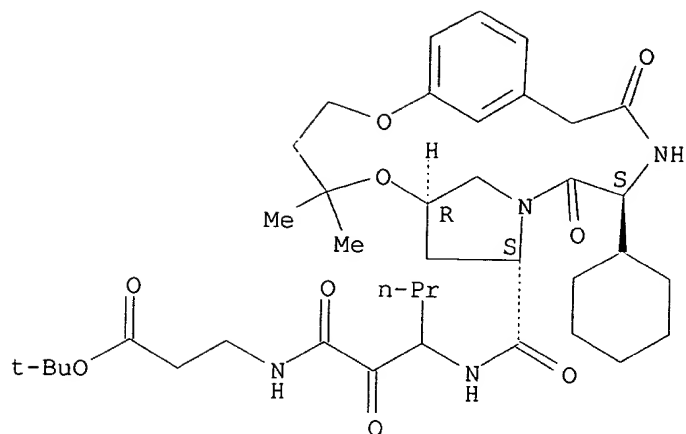
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 17 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367258-20-6 REGISTRY
 CN .beta.-Alanine, (2S)-2-cyclohexyl-N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]glycyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-oxohexanoyl-, 1,1-dimethylethyl ester, cyclic (1.fwdarw.2)-ether (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C39 H58 N4 O9
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



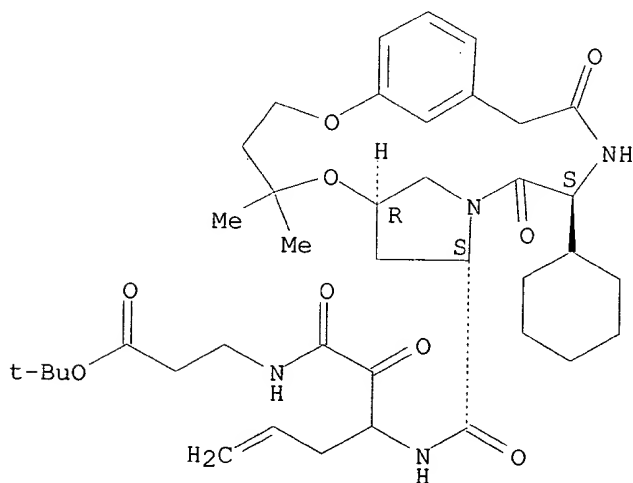
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 18 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-19-3 REGISTRY
CN .beta.-Alanine, (2S)-2-cyclohexyl-N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]glycyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-oxo-5-hexenoyl-, 1,1-dimethylethyl ester, cyclic (1.fwdarw.2)-ether (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C39 H56 N4 O9
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



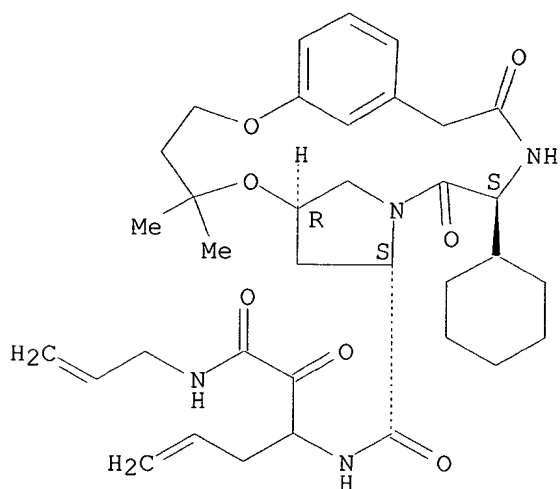
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 19 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-18-2 REGISTRY
CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, 12-cyclohexyl-5,5-dimethyl-11,14-dioxo-N-[1-[oxo(2-propenylamino)acetyl]-3-butenyl]-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C35 H48 N4 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



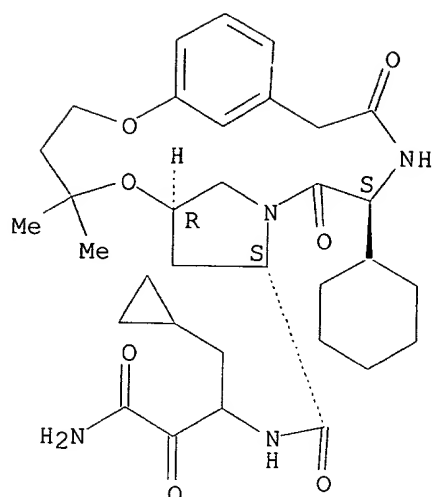
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 20 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-17-1 REGISTRY
CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, N-[3-amino-1-(cyclopropylmethyl)-2,3-dioxopropyl]-12-cyclohexyl-5,5-dimethyl-11,14-dioxo-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H46 N4 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



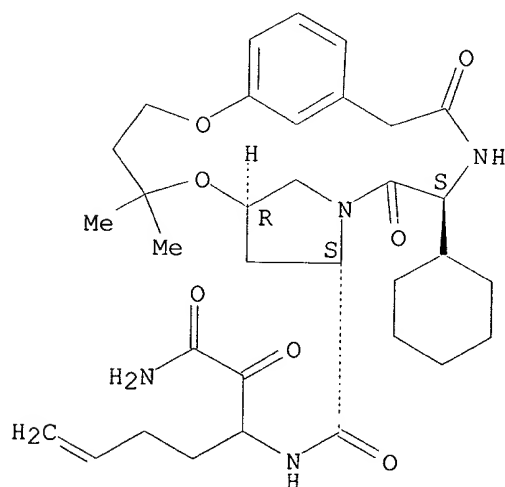
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 21 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-16-0 REGISTRY
CN 2,6-Dioxo-10,13-diazatriene-1(20),16,18-triene-9-carboxamide, N-[1-(aminooxoacetyl)-4-pentenyl]-12-cyclohexyl-5,5-dimethyl-11,14-dioxo-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H46 N4 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



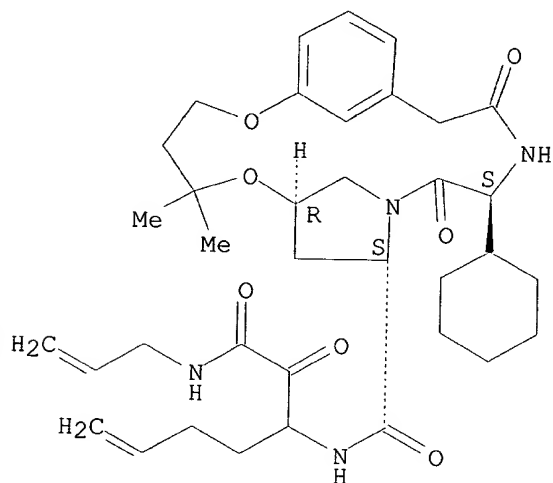
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 22 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367258-15-9 REGISTRY
 CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, 12-cyclohexyl-5,5-dimethyl-11,14-dioxo-N-[1-[oxo(2-propenylamino)acetyl]-4-pentenyl]-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C36 H50 N4 O7
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



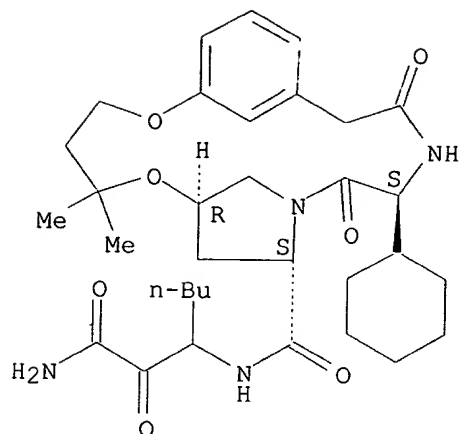
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 23 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367258-14-8 REGISTRY
 CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, N-[1-(aminooxoacetyl)pentyl]-12-cyclohexyl-5,5-dimethyl-11,14-dioxo-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C33 H48 N4 O7
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



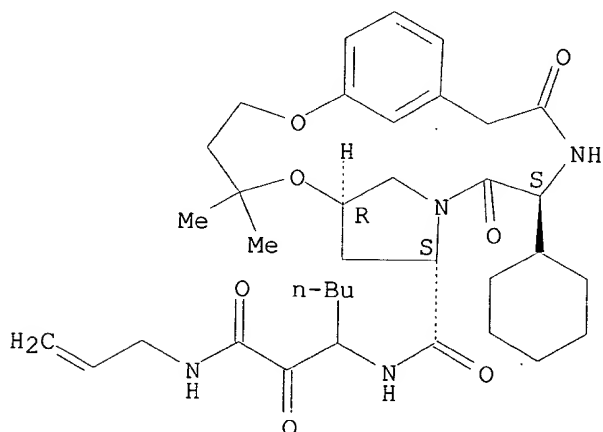
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 24 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-13-7 REGISTRY
CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamidé, 12-cyclohexyl-5,5-dimethyl-11,14-dioxo-N-[1-[oxo(2-propenylamino)acetyl]pentyl]-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C36 H52 N4 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

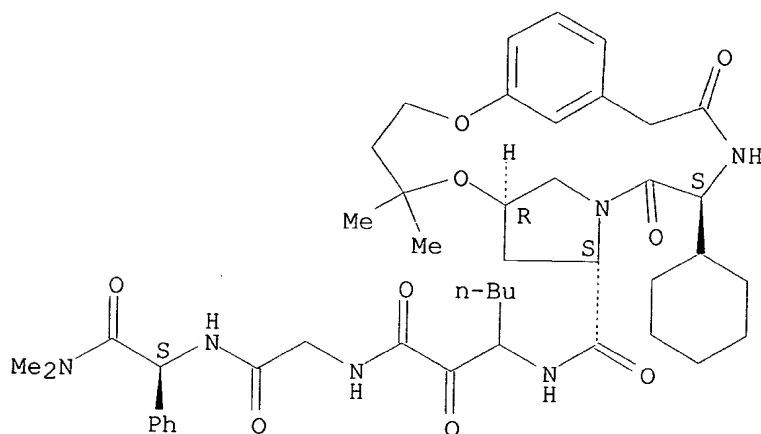
1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 25 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367258-12-6 REGISTRY
 CN Glycinamide, (2S)-2-cyclohexyl-N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]glycyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-oxoheptanoylglycyl-N,N-dimethyl-2-phenyl-, cyclic (1.fwdarw.2)-ether, (2S)- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C45 H62 N6 O9
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



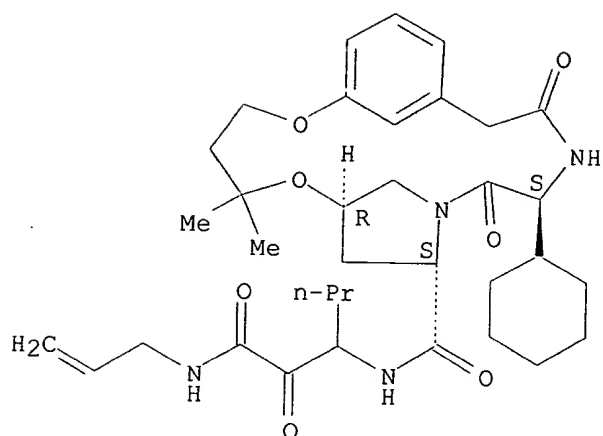
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 26 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367258-11-5 REGISTRY
 CN 2,6-Dioxo-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, 12-cyclohexyl-5,5-dimethyl-11,14-dioxo-N-[1-[oxo(2-propenylamino)acetyl]butyl]-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C35 H50 N4 O7
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



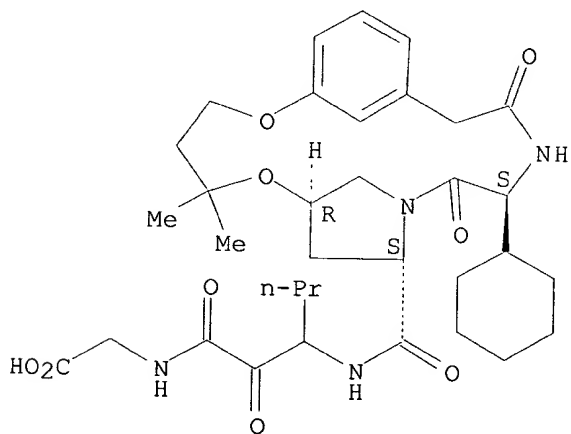
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 27 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-10-4 REGISTRY
CN Glycine, (2S)-2-cyclohexyl-N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]glycyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-oxohexanoyl-, cyclic (1.fwdarw.2)-ether (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C34 H48 N4 O9
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



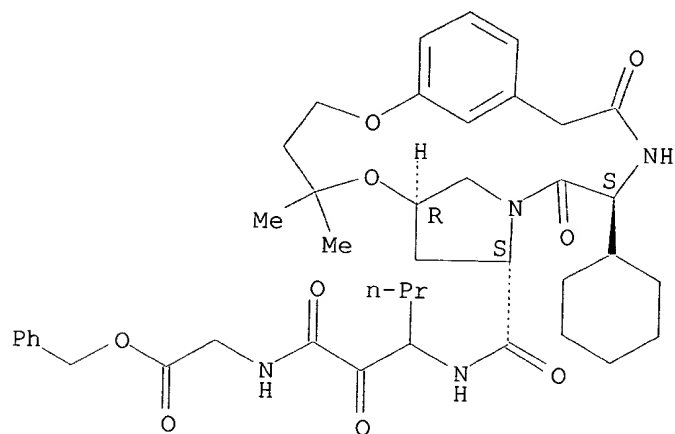
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 28 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367258-09-1 REGISTRY
 CN Glycine, (2S)-2-cyclohexyl-N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]glycyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-oxohexanoyl-, phenylmethyl ester, cyclic (1.fwdarw.2)-ether (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C41 H54 N4 O9
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



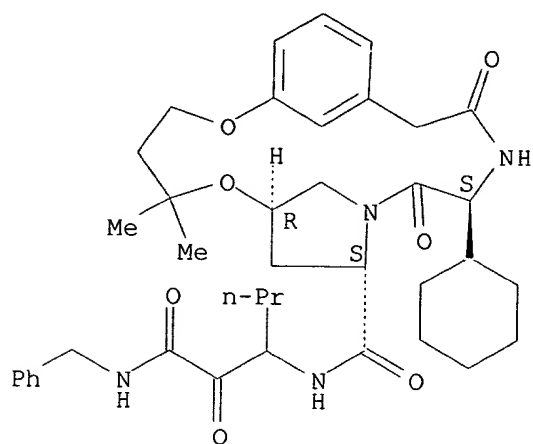
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 29 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367258-08-0 REGISTRY
 CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, 12-cyclohexyl-5,5-dimethyl-11,14-dioxo-N-[1-[oxo[(phenylmethyl)amino]acetyl]butyl]-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C39 H52 N4 O7
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

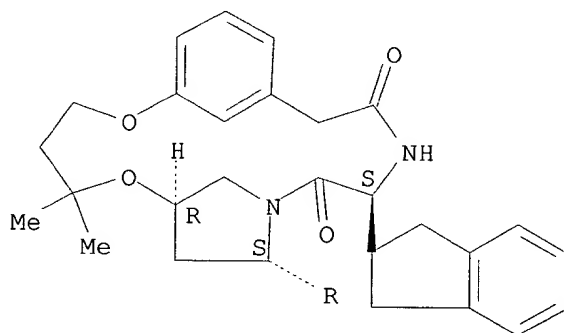
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REFERENCE 1: 135:318715

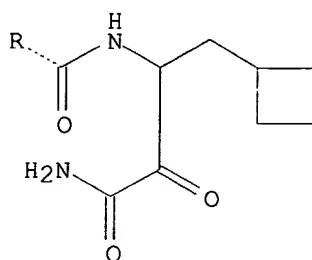
L3 ANSWER 30 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367258-03-5 REGISTRY
CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxamide, N-[3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-12-(2,3-dihydro-1H-inden-2-yl)-5,5-dimethyl-11,14-dioxo-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C37 H46 N4 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

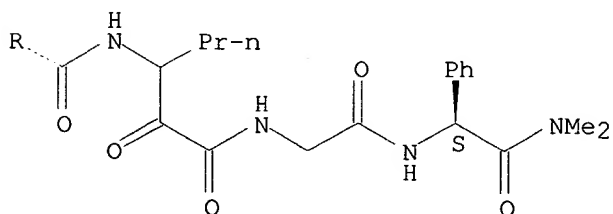
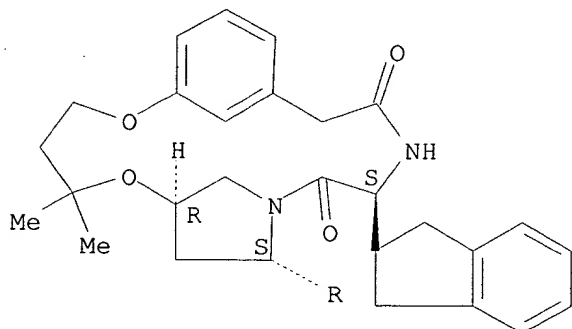
1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 31 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367257-96-3 REGISTRY
CN Glycinamide, (2S)-2-(2,3-dihydro-1H-inden-2-yl)-N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]glycyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-oxohexanoylglycyl-N,N-dimethyl-2-phenyl-, cyclic (1.fwdarw.2)-ether, (2S)-(9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C47 H58 N6 O9
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

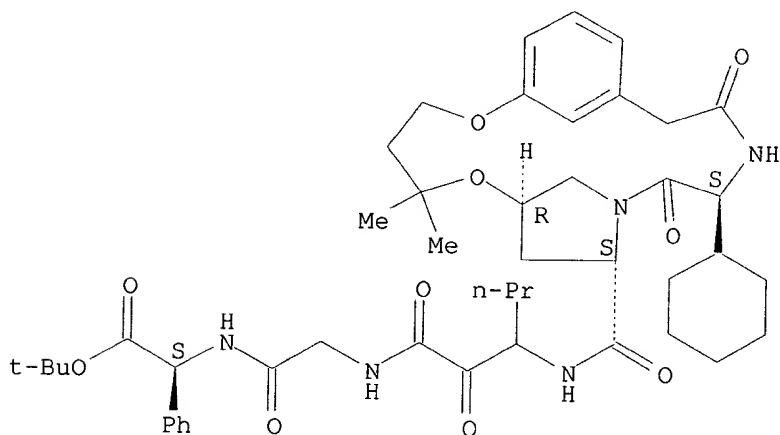
1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 32 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367257-62-3 REGISTRY
CN Glycine, (2S)-2-cyclohexyl-N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]glycyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-oxohexanoylglycyl-2-phenyl-, 1,1-dimethylethyl ester, cyclic (1.fwdarw.2)-ether, (2S)- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C46 H63 N5 O10
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

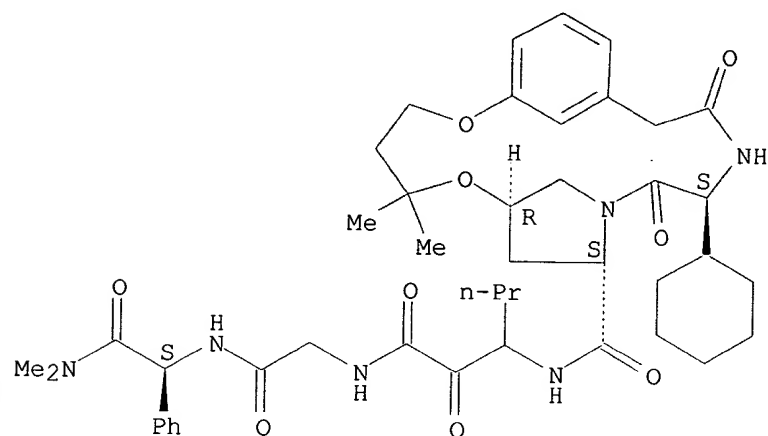
1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

L3 ANSWER 33 OF 33 REGISTRY COPYRIGHT 2003 ACS on STN
RN 367257-61-2 REGISTRY
CN Glycinamide, (2S)-2-cyclohexyl-N-[[3-(3-hydroxy-3-methylbutoxy)phenyl]acetyl]glycyl-(4R)-4-hydroxy-L-prolyl-3-amino-2-oxohexanoylglycyl-N,N-dimethyl-2-phenyl-, cyclic (1.fwdarw.2)-ether, (2S)- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C44 H60 N6 O9
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)

1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715

=> fil hcaplus
 FILE 'HCAPLUS' ENTERED AT 18:58:27 ON 29 JUL 2003
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 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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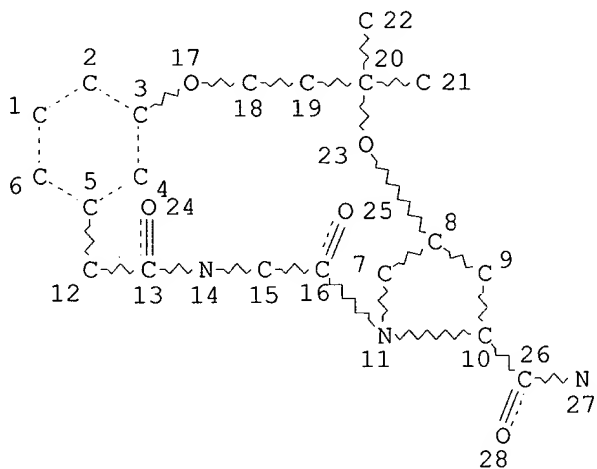
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FILE COVERS 1907 - 29 Jul 2003 VOL 139 ISS 5
 FILE LAST UPDATED: 28 Jul 2003 (20030728/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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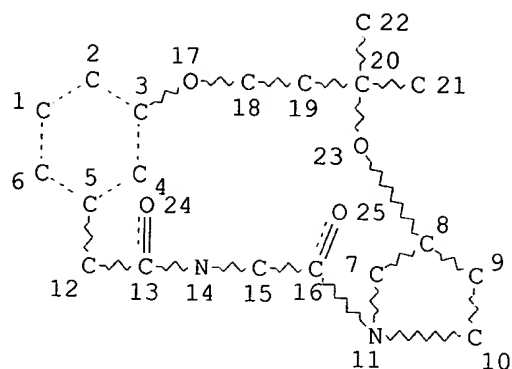
=> d stat que 19
 L1 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE
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 L4 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L3
 L5 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 25

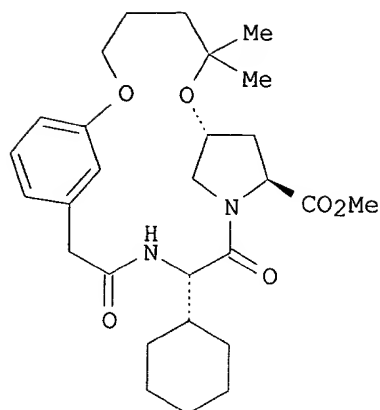
STEREO ATTRIBUTES: NONE

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 L8 2 SEA FILE=REGISTRY ABB=ON PLU=ON L7 NOT L3
 L9 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L8 NOT L4

=>
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=> d ibib abs hitrn 19 1

L9 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2002:221307 HCAPLUS
 DOCUMENT NUMBER: 136:386105
 TITLE: Syntheses of Novel 4-tert-Alkyl Ether Proline-Based
 16- and 17-Membered Macrocyclic Compounds
 AUTHOR(S): Chen, Kevin X.; Njoroge, F. George; Vibulbhan, Bancha;
 Buevich, Alexei; Chan, Tze-Ming; Girijavallabhan,
 Viyyoor
 CORPORATE SOURCE: Schering-Plough Research Institute, Kenilworth, NJ,
 07033, USA
 SOURCE: Journal of Organic Chemistry (2002), 67(8), 2730-2733
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



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AB Starting from N-Cbz-4-hydroxyproline Me ester, a boron trifluoride-diethyl etherate-catalyzed reaction provided 4-tert-alkyl ether proline. Two deprotections and amide bond formations furnished a phenol alc. Macrocyclization was accomplished through a Mitsunobu reaction using triphenylphosphine and 1,1'-(azodicarbonyl)dipiperidine to afford novel 16- and 17-membered proline-based macrocyclic compds. of type, e.g., I.

IT **367261-09-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of 4-tert-alkyl ether proline-based 16- and 17-membered macrocyclic compds.)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>
=>

=> fil reg

FILE 'REGISTRY' ENTERED AT 18:58:48 ON 29 JUL 2003
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 JUL 2003 HIGHEST RN 556740-18-2
DICTIONARY FILE UPDATES: 28 JUL 2003 HIGHEST RN 556740-18-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

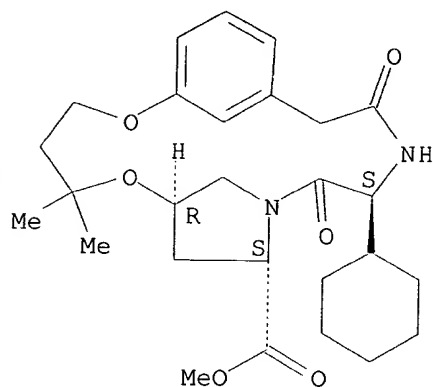
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>
=>

=> d ide can 18 1-2

L8 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367261-09-4 REGISTRY
 CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxylic acid, 12-cyclohexyl-5,5-dimethyl-11,14-dioxo-, methyl ester, (7R,9S,12S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C27 H38 N2 O6
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

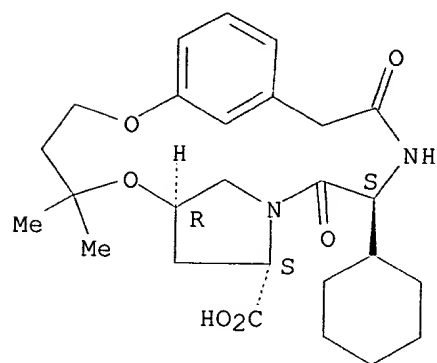
2 REFERENCES IN FILE CA (1947 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 136:386105

REFERENCE 2: 135:318715

L8 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 367259-03-8 REGISTRY
 CN 2,6-Dioxa-10,13-diazatricyclo[14.3.1.17,10]heneicosa-1(20),16,18-triene-9-carboxylic acid, 12-cyclohexyl-5,5-dimethyl-11,14-dioxo-, (7R,9S,12S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C26 H36 N2 O6
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1: 135:318715